Interface characterisation and internal electric field evaluation of a-Si:H pin solar cell by variable energy positron annihilation spectroscopy

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INTERFACE CHARACTERISATION AND INTERNAL ELECTRIC FIELD
EVALUATION OF a-Si:H PIN SOLAR CELL BY VARIABLE ENERGY POSITRON
ANNIHILATION SPECTROSCOPY

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ABSTRACT

By means of the slow positron beam Doppler-broadening technique, the depth profile of
microvoids across a p-i-n double junction solar cell has been resolved. VEPFIT fitting results
indicate an approximately uniform density of the defects throughout the solar cell, but with an
enhanced concentration at all of the interfaces possibly due to network mismatch. In order to
evaluate the internal electric field, Variable Energy Positron Annihilation Spectroscopy
(VEPAS) measurements have been performed on a single junction pin solar cell at different
biases. The internal electric field effect on positrons has also been examined in terms of the bias
dependence of positron drift in a-Si:H single junction pin solar cell.

INTRODUCTION

In order to achieve a higher conversion efficiency, it is necessary to obtain more detailed
information about physical quantities influencing solar cell performance. As has been remarked
elsewhere, the main transport mechanism of photogenerated carriers in an a-Si:H solar cell is
drift. Under such a circumstance, the magnitude of the internal electric field in the i-layer and
interface properties have a direct effect on carrier collection and transport. In this sense, it is
worth knowing the profile of the internal electric field and the interface characteristics in an
actual a-Si:H solar cell. As conventional methods to determine internal field are not useful in a
pin junction solar cell due to the spread of the space charge region throughout the i-layer, we
propose here a new method, positron annihilation spectroscopy, to perform the characterisation
and evaluation of the internal electric field in a-Si:H solar cells.

EXPERIMENTAL DETAILS

Samples Description

The samples in this work were a double-junction a-Si:H pin/pin and a single-junction solar
cell deposited by conventional glow discharge and covered with 400nm-thick and 600nm-thick
Au electrodes respectively. Positrons were implanted from the Au electrode side in both samples.
The configuration of the pin/pin double-junction solar cell was Au/n'-i-p'/n'-i-p'/ITO/glass and
that of pin single-junction one was Au/n'-i-p'/ITO/glass. The performance of the solar cells was
verified by diode output properties, showing that both solar cells had good characteristics. In this
paper, the double-junction pin/pin solar cell was used without bias to characterise microvoids
across the whole device, and the single-junction cell with bias for internal field examination.
Variable Energy Positron Beam Annihilation Experiment

The positron beam annihilation experiment consisted of implanting positrons of controlled energy into a zero biased contact in the double junction a-Si:H pin/pin solar cell, and into a positively (negatively) biased contact such that the internal electric field direction was parallel (anti-parallel) to the direction of positron injection, so as to cause positron drift into the cell (back to the Au/n interface), in the single-junction a-Si:H pin solar cell, as well. The positron annihilation spectroscopy measurements were carried out using the magnetically guided positron beam at The University of Hong Kong which has been described elsewhere [1]. The intensity of the slow positron beam was about $1 \times 10^4$ e$^+$/s, and its diameter was 6mm. The incident-beam energy was varied from 0.15-25KeV in steps of 250eV. The variation of the beam energy allows control over the mean depth of positron implantation into the samples. In general, the mean penetration depth of the positrons implanted at energy $E$ can be determined from [2] $x_0 = A E^n$, where the constant $A$ has been found empirically to be $\sim 400/\rho \AA/\text{KeV}^n$, $\rho$ is the sample density in g/cm$^3$, $x_0$ is in $\AA$, $E$ is in KeV, and the power $n \approx 1.6$ for most materials [2, 3]. Thus for a-Si:H ($\rho=2.2 \text{g/cm}^3$) the maximum positron beam energy 25KeV employed in the present study corresponds to a mean positron stopping depth of about 3$\mu$m. This energy range was chosen so that at an intermediate positron implantation energies all positrons essentially annihilate in the a-Si:H pin solar cells while at the highest energies almost full penetration into the glass substrate could be achieved thus allowing depth profiling across the entire sample.

The 511 KeV annihilation $\gamma$ spectra were detected and accumulated by a high purity Ge detector of resolution 1.4KeV at 514KeV and a digitally stabilised multichannel analyser system. A total of $1 \times 10^6$ counts were collected under the annihilation photopeak for each positron energy. The photopeak line shape of $\gamma$-rays was described using the conventional valence and core annihilation parameters $S$ and $W$, which are the ratios of counts in the central and wing portions of the annihilation photopeak to the total counts in the 511KeV peak, respectively [2]. $S$-parameter versus implantation energy spectra were taken with the Au contact at -2V, 0V, and 2V for the a-Si:H pin single junction solar cell and 0V for the double junction a-Si:H solar cell.

RESULTS AND DISCUSSIONS

Positrons get trapped at neutral and negative vacancy defects because the missing positive charge of the ion cores causes the particle to experience a potential well. With increasing number of microvoids, the valence annihilation parameter $S$ increases and the core annihilation parameter $W$ decreases. A trapped positron at a vacancy overlaps mainly with the core electrons of the nearest neighbour atoms. Hence the shape and magnitude of the core electron momentum distribution can be used to identify the vacancy acting as a positron trap.

Interface Characterisation In a-Si:H pin/pin Double Junction Solar Cell

VEPAS was carried out on the a-Si:H double junction pin/pin solar cell to evaluate the interface characteristics. Figure 1 shows the measured data and VEPFIT fit. The measured $S$ parameter is about 0.427 at low positron implantation energy. This is attributed to positrons annihilating on or close to the surface. As the implanting energy increases, more positrons annihilate in the Au overlayer and this results in the decrease of the $S$-parameter to a value of about 0.419. The $S$-parameter increases with further increase of positron implantation energy as more positrons annihilate in the bulk of the diode. The $S$-parameter moves to the $p'$/ITO
interface, increases afterwards and finally approaches a value corresponding to the ITO/glass interface. Thus the internal interfaces of the double junction pin/pin solar cell do not affect the S-parameter, indicating there is no large density of voids at the interfaces and hence that the interfaces are of good quality, in agreement with the conclusion drawn from the good diode characteristics measured.

![Graph](image)

Figure 1. The line shape parameter S as a function of incident positron energy for a-Si:H double junction solar cell. The circles are for VEPAS results and solid line for VEPFIT results.

To confirm the results above, an S/W-E plot has been drawn in figure 2. S/W parameter can distinguish the surface annihilation from the bulk annihilation mode more clearly than S, because the surface annihilation mode gives a very low value for W. A flatter trend of S/W is seen, except at the Au/n' interface, and in particular at the p'/ITO interface, again implying good internal interface quality.

**Microvoids Contents Evaluation**

To fit the S parameter profiles, a 5-layered model, representing the Au/n', i-layer, p'/n', i-layer, and p'/ITO/glass layers, was adopted to represent the double junction solar cell. Assuming a uniform defect profile in each slab, the positron trapping rate in the defects is related to the effective positron diffusion length by [2]

\[
\mu C_{vac} = \frac{D_\gamma}{L_{\gamma,eff}^2} - \lambda_b
\]  

(1)

where \(D_\gamma\) is the positron diffusion coefficient, \(\lambda_b\) the free-positron annihilation rate, \(\mu\) the specific trapping rate by vacancies, \(C_{vac}\) the vacancy concentration, and \(L_{\gamma,eff}\) the effective diffusion length of positron in the material.

The vacancy concentration can thus be found using equation (1) given \(L_{\gamma,eff}\). The effective diffusion length of positrons in the device were found to be, by VEPFIT, 6.7nm, 15.4nm, 10.3nm, 16.2nm, and 4.8nm for slabs of Au/n', i-layer, p'/n', i-layer, and p'/ITO/glass,
respectively. Adopting values for crystalline Si [2], of $\mu=3 \times 10^{14}\text{s}^{-1}$, $D_s=2.2\text{cm}^2\text{s}^{-1}$, and $\lambda_v=4.59\times10^8\text{s}^{-1}$ (divacancies), we obtain void concentration of $1.6\times10^2$ atomic fraction (at.fr.) in the Au/n$^+$ region, $3.1\times10^3$ at.fr. for the i-layer in the bottom cell, $6.9\times10^3$ at.fr. for the p$^+/n^+$ interconnection, $2.8\times10^3$ at.fr. for the i-layer in the top cell, and $3.2\times10^3$ at.fr. for the p$^+/\text{ITO/glass}$ region. Again using c-Si data the diffusion coefficient of positrons was taken as $D=2.2\text{cm}^2\text{s}^{-1}$. The annihilation rate, corresponding to crystalline Si divacancies, was taken as $\lambda_v=4.59\times10^8\text{s}^{-1}$ [2]. These results clearly demonstrate that the microvoid fraction at the internal p$^+/n^+$ intercell interface and both intrinsic active layers are low, but those at the p$^+/\text{ITO}$ and Au/n$^+$ interfaces are quite high, indicating that good internal interface quality is most important for a good device performance.

![Graph](image)

Figure 2. The S/W parameter as a function of incident positron energy for a-Si:H double junction solar cell.

**Internal Electric Field Effects In a-Si:H pin Single Junction Solar Cell**

VEPAS study of an a-Si:H pin solar cell displayed sensitivity of positrons to interface trap centres. A natural extension of this study is to examine the internal electric field profile in the intrinsic region and that at the interfaces. Since positrons are themselves charged, they are influenced by the electric field in the solar cell very much like normal charge carriers. However, although positrons and holes carry the same unit of charge, their motion in an electric field is governed by fundamentally different mechanisms.

Figure 3 is a plot of the S parameter, under different bias voltage V, as a function of positron implantation energy, for the single junction a-Si:H pin solar cell. The S parameter is a linear sum of contributions from all layers, i.e., the Au contact, n$'/i$ interface, bulk intrinsic active i layer, i/p$'$ interface, and p$'/\text{ITO/glass}$ region, which may be written,

$$S = F_{\text{Au}}S_{\text{Au}} + F_{p'/\text{ITO/glass}}S_{p'/\text{ITO/glass}} + F_{n'/i}S_{n'/i} + F_{i/p}S_{i/p} + F_iS_i$$

(2)

where F denotes the fraction of positrons annihilating in different layers. The first two terms are nearly constant for all bias voltages, but the sum $F_{n'/i}S_{n'/i} + F_{i/p}S_{i/p} + F_iS_i$ changes with the bias.

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voltage. Depending on the polarity and strength of the external and internal field, the fraction of positrons annihilating at the n'/$i$ and i/p' interfaces and bulk i layer can vary, although their sum $F_{n/i} + F_{i/p'} + F_i$ is a constant.

![Graph showing S parameter vs. Positron Beam Incident Energy (KeV) with different bias voltages.]

**Figure 3.** A plot of the S parameter, under different bias voltage $V$, as the function of positron implantation energy, for a-Si:H pin solar cell.

At negative applied voltage, more positrons drift to the $n'/i$ interface, so that the measured S parameter will exhibit a stronger interface character. Suppose $S_{n/i}$ and $S_{i/p'}$ are constants like $S_i$. From the measurements on the double junction solar cell, we know that $S_{n/i}$ and $S_{i/p'}$ are greater than $S_i$. When the bias voltage $V$ increases from a negative to a positive value, $F_{n/i}$ and $F_{i/p'}$ decrease monotonically with a corresponding increase in $F_i$. Since $S_{n/i}$ and $S_{i/p'}$ are greater than $S_i$, the trend of the linear sum $F_{n/i}S_{n/i} + F_{i/p'}S_{i/p'} + F_iS_i$ depends on the variation of fraction of positrons annihilating at interfaces and intrinsic active layer with the variation of the sum internal electric field. Figure 3 indicates experimentally that there is a monotonic decrease in S parameter while the bias voltage is approaching a positive value (+2V), implying the positron annihilation at both the $n'/i$ and i/p' interfaces governs the annihilation process in a-Si:H pin single junction solar cells due to the internal electric field in the vicinity of the interfaces.

For a +2V positive bias, the sum internal field points away from the Au contact and, therefore, implanted positrons drift towards the intrinsic active layer, so increasing $F_i$ and decreasing $F_{n/i}$ and $F_{i/p'}$. Hence $S_i$ dominates the measured S value, as shown in figure 3 at smaller implantation energy. But at the i/p' interface, the positron annihilation displayed is less than that in the unbiased sample, due to positron movement towards the i/p' interface under the influence of the field.

Subtracting the S-parameter of the unbiased S spectrum from the biased spectra, we obtained the variation in S resulting from bias, which is plotted in figure 4. It is noted that bumps exist mainly at the interfaces so that the electric field effects on positron annihilation in a-Si:H pin solar cells are dramatic. These arguments suggest that the internal electric field can be extracted quantitatively by VEPAS measurements, by a numerical solution of the diffusion equation of positrons in the presence of a field. This work is now being undertaken.
Figure 4. Differences of S-parameters comparing with that of unbiased a-Si:H pin solar cell. Lines are drawn for eyes.

CONCLUSIONS

In summary, we have carried out positron annihilation measurements on an a-Si:H pin/pin double junction solar cell at zero bias and on an a-Si:H pin single junction solar cell at several different biases. By means of the slow positron beam Doppler-broadening technique, the microvoids concentration across the pin/pin double junction solar cell has been resolved. VEPFIT fitting results indicated an approximately uniform density of the defects throughout the solar cell, but with an enhanced concentration at all of the interfaces possibly due to network mismatch. For the evaluation of the internal electrical field in the a-Si:H pin single junction solar cell, variable energy positron annihilation spectroscopy measurements have been performed over positron energies of 0–25KeV. A clear effect of bias was seen in the S-parameter spectra, in particular in the vicinity of the p+/i and n+/i interfaces. It is expected that suitable numerical fitting will be able to produce quantitative field profile from such measurements in the future.

REFERENCE

